



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 05:21 AM 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 validation summary 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/ValidationPDFNotes.html>

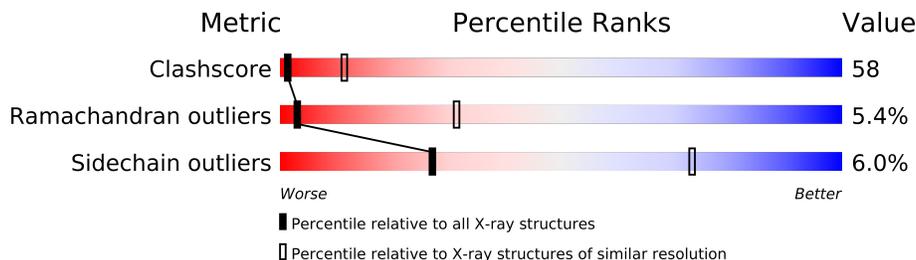
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	79885	1214 (3.50-3.30)
Ramachandran outliers	78287	1177 (3.50-3.30)
Sidechain outliers	78261	1177 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 hydrogen and 0 are deuterium.

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.

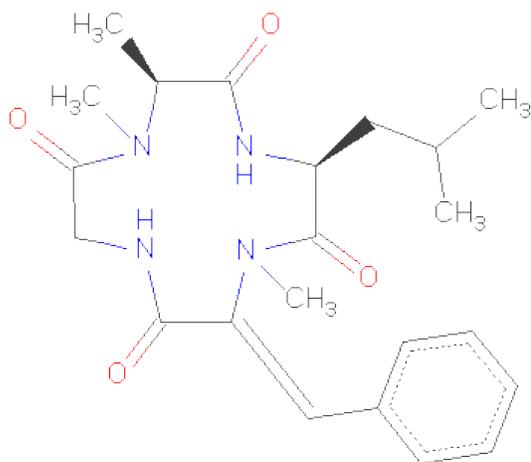
- Molecule 1 is a protein called ATPase alpha subunit.

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

- Molecule 2 is a protein called ATPase beta subunit.

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

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



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

L469	L480	K392	S320	L186	R122
P470	D481	E393	I321	M187	P123
E471	E482	T394	T322	M188	
A472	A483	L395	S323	A190	T126
F474	A484	Q396	I324	Y259	T128
Y475	E485	R397	Q325	F260	T129
L476		Y398	A326	R261	S130
V477		K399	Y327	R262	P131
		E400	Y328	V263	H133
		L401	V329	N264	H132
		Q402	D333	E265	R134
		D403	L334	Q266	R135
		L404	T335	D267	A136
		I405	A338	V268	P137
		A406	A338	L269	A138
		T407	L269	L270	F139
LYS		G409	T341	L271	E204
ALA		L410	T342	T272	R205
MET		D411	F343	D273	O141
ASN		E412	A344	N274	L142
LEU		L413	H345	L275	E208
GLU		S414	L346	F276	T144
MET			D347	R277	K145
GLU			D417	F278	L146
SER			R418	V279	S147
LYS			L419	Q280	L148
LEU			T420	Q281	F149
LYS			V421	G282	
LYS			A422	S283	G152
			R423	E284	I153
			A424	V285	K154
			R425	S286	V155
			K426	A287	V156
			L427	L288	M157
			E428	L289	L158
			R429	A364	A160
			F430	P367	P161
			L431	L368	Y162
			S432	D369	R163
			Q433	Y298	R164
			P434	Q299	G165
			F435	P300	G166
			A438	T373	K167
			L451	M374	I168
			T454	L375	G169
			L455	Q376	M239
				P377	R240
				R378	L170
				I379	F171
				V380	
				G381	G175
				Y385	V176
				L460	K178
				L461	R246
				L462	M247
				S463	R248
				G464	V180
				E465	V249
				L466	G250
					L251
					T252
					E184
					M183
					I182
					V179
					G177
					A245
					G244
					P243
					E241
					P242
					R246
					K231
					V232
					A233
					L234
					Y235
					G237
					Q236
					T222
					V221
					G220
					S219
					M216
					L212
					T206
					R207
					L144
					E209
					G209

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, α , β , γ	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 ²)	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 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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 58.

The worst 5 of 844 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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%)	3	30
2	B	465/498 (93%)	365 (78%)	76 (16%)	24 (5%)	3	32
All	All	940/1005 (94%)	727 (77%)	162 (17%)	51 (5%)	3	31

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 [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%)	367 (95%)	21 (5%)	31 77
2	B	381/410 (93%)	356 (93%)	25 (7%)	24 70
All	All	769/824 (93%)	723 (94%)	46 (6%)	27 73

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
2	B	42	ASN
2	B	60	ASN

5.3.3 RNA [i](#)

There are no RNA chains 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)

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	3.21	8 (25%)	43,43,43	3.89	12 (27%)

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TTX	B	499	2	-	0/45/45/45	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	O1-C6	11.38	1.43	1.22
3	B	499	TTX	C15-C14	-8.11	1.33	1.50
3	B	499	TTX	C6-N1	5.34	1.45	1.35
3	B	499	TTX	C5-C6	5.07	1.64	1.53
3	B	499	TTX	C7-N1	-3.99	1.38	1.47

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	499	TTX	C5-C6-N1	-14.89	91.91	118.84
3	B	499	TTX	C7-N1-C6	-14.23	95.53	118.82
3	B	499	TTX	C4-C5-C6	6.94	121.72	109.37
3	B	499	TTX	C6-N1-C15	6.66	141.30	123.69
3	B	499	TTX	C13-N4-C14	5.38	130.12	121.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.