



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 06:42 am BST

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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	<b>NOT EXECUTED</b>
EDS	:	<b>NOT EXECUTED</b>
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

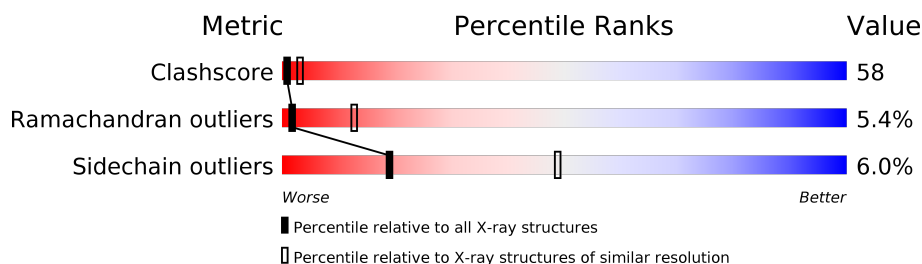
# 1 Overall quality at a glance

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	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)

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 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 [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.

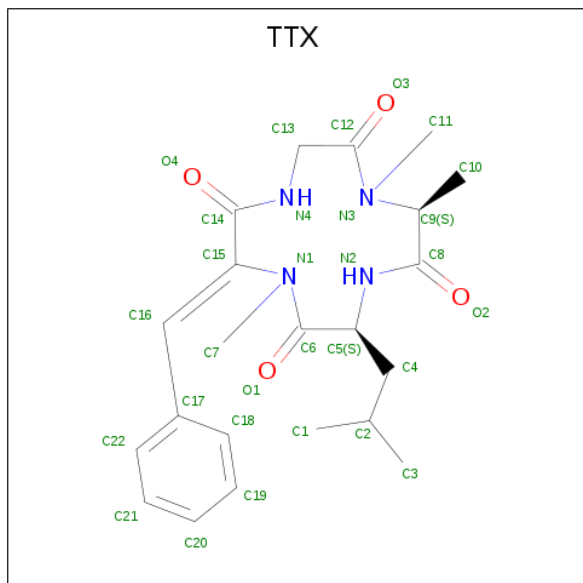
- Molecule 1 is a protein called ATPase alpha subunit.

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:  $C_{22}H_{30}N_4O_4$ ).



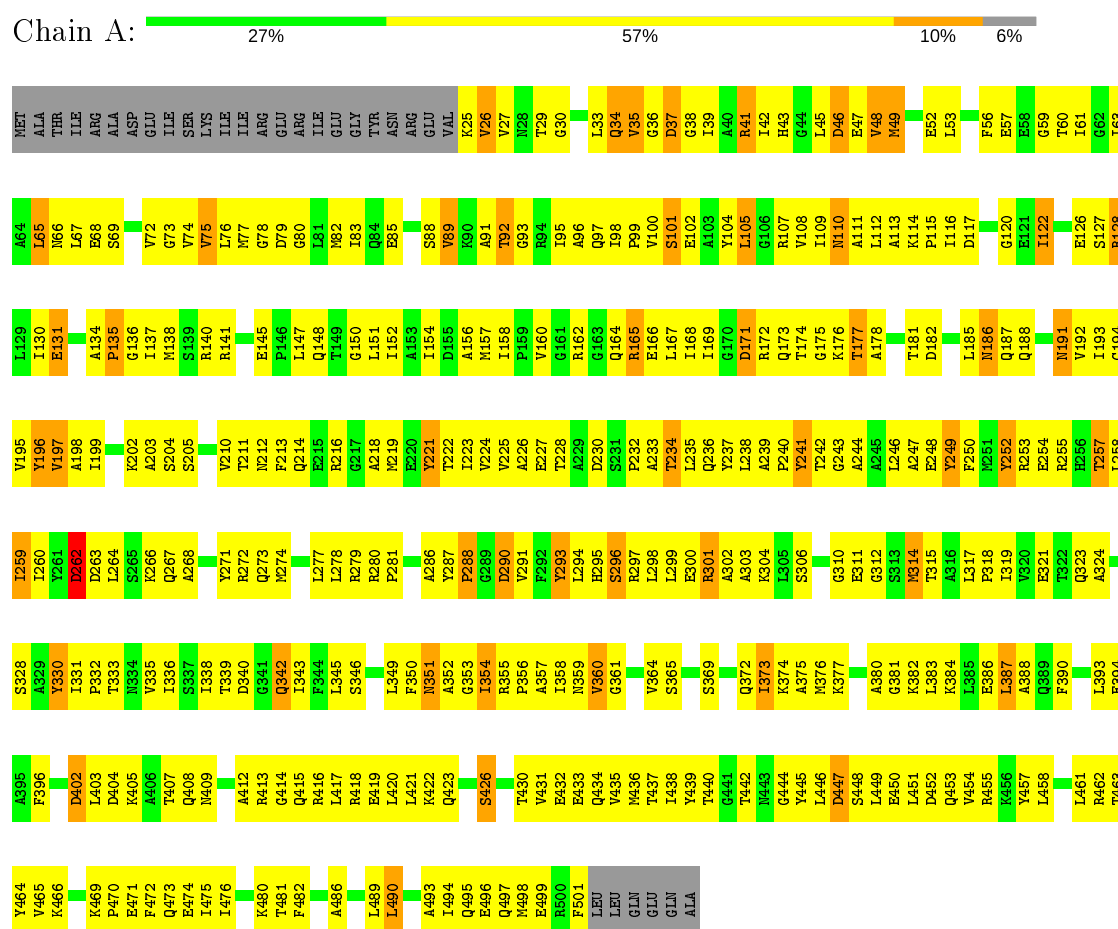
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			30	22	4	4		

### 3 Residue-property plots

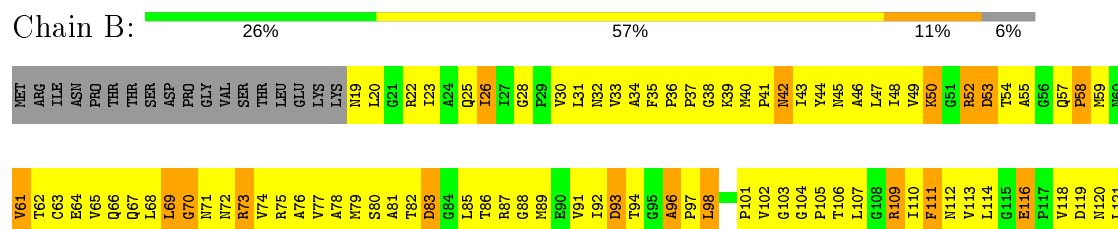
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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	T256	P123	
E471	T394	S322	M256		
	L395	S323	A257	T126	
Q472	Q396	I324	E258	R127	
A473	R397	Q325	Y259	T128	
F474	Y398	A326	F260	T129	
Y475	K399	Y327	R261	S130	
L476	E400	Y328	D262	P131	
V477	L401	V329	V263	H132	
	Q402		N264	S197	
I480	D403	D333	E265	R134	
D481	I404	L334	Q266	S135	
E482	I405	T335	L267	A136	
A483	A406		V268	P137	
	I407	A338	L269	A138	
I485	L408		L270	F139	
LYS	G409	T341	F271	T140	
ALA	L410	T342	I272	Q141	
NET	D411	F343	D273	L142	
ASN	E412	A344	N274	D143	
LEU	L413	H345	I275	T144	
GLU	S414	L346	F276	K145	
		D347	R277	L146	
NET			F278	S147	
GLU	D417		V279	I148	
SER	R418	T350	Q280	F149	
LYS	L419	V351	A281		
LEU	T420	L352	G282		
LYS	V421	S353	S283	G152	
	A422		E284	I153	
	R423	L356	V285	K154	
	A424	A357	S286	V155	
R425			A287	V156	
K426		I361	L288	N157	
I427		Y362	L289	L158	
P428		P363	G289	I159	
R429		A364	E290	A160	
F430			R291	P161	
L431		P367		Y162	
S432		L368	V296	R163	
Q433		D369	G297	R164	
P434			Y298	G165	
F435		S372	Q299	G166	
		T373	P300	K167	
		M374	T301	L168	
		L375	L302	G169	
		Q376		L170	
		P377	E305	F171	
		R378			
		I379	S308	G175	
		V380	L309	V176	
		G381	Q310	G177	
			A245	K178	
			R246	T179	
		Y385	E311	V180	
		E386	R312	L181	
		I461	I313	I182	
		L462	T314	M183	
		I387	S315	E184	
		A388	T316	L185	
		S463			
		G464	G319		
		E465			
		L466			

## 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, $\alpha$ , $\beta$ , $\gamma$	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 5.0, CNS	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%)	1	12
2	B	465/498 (93%)	365 (78%)	76 (16%)	24 (5%)	2	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	940/1005 (94%)	727 (77%)	162 (17%)	51 (5%)	2	13

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%)	22	52
2	B	381/410 (93%)	356 (93%)	25 (7%)	16	46
All	All	769/824 (93%)	723 (94%)	46 (6%)	19	49

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	3.37	9 (29%)	40,43,43	4.35	13 (32%)

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	-	15/45/45/45	0/1/2/2

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	499	TTX	O1-C6	11.81	1.43	1.22
3	B	499	TTX	C15-C14	-7.80	1.33	1.49
3	B	499	TTX	C6-N1	6.10	1.45	1.35
3	B	499	TTX	C5-C6	5.71	1.64	1.53
3	B	499	TTX	C7-N1	-4.42	1.38	1.47

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	499	TTX	C5-C6-N1	-16.65	91.91	118.78
3	B	499	TTX	C7-N1-C6	-16.32	95.53	118.81
3	B	499	TTX	C4-C5-C6	6.59	121.72	109.35
3	B	499	TTX	C6-N1-C15	6.44	141.30	123.52
3	B	499	TTX	C13-N4-C14	5.66	130.12	121.25

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

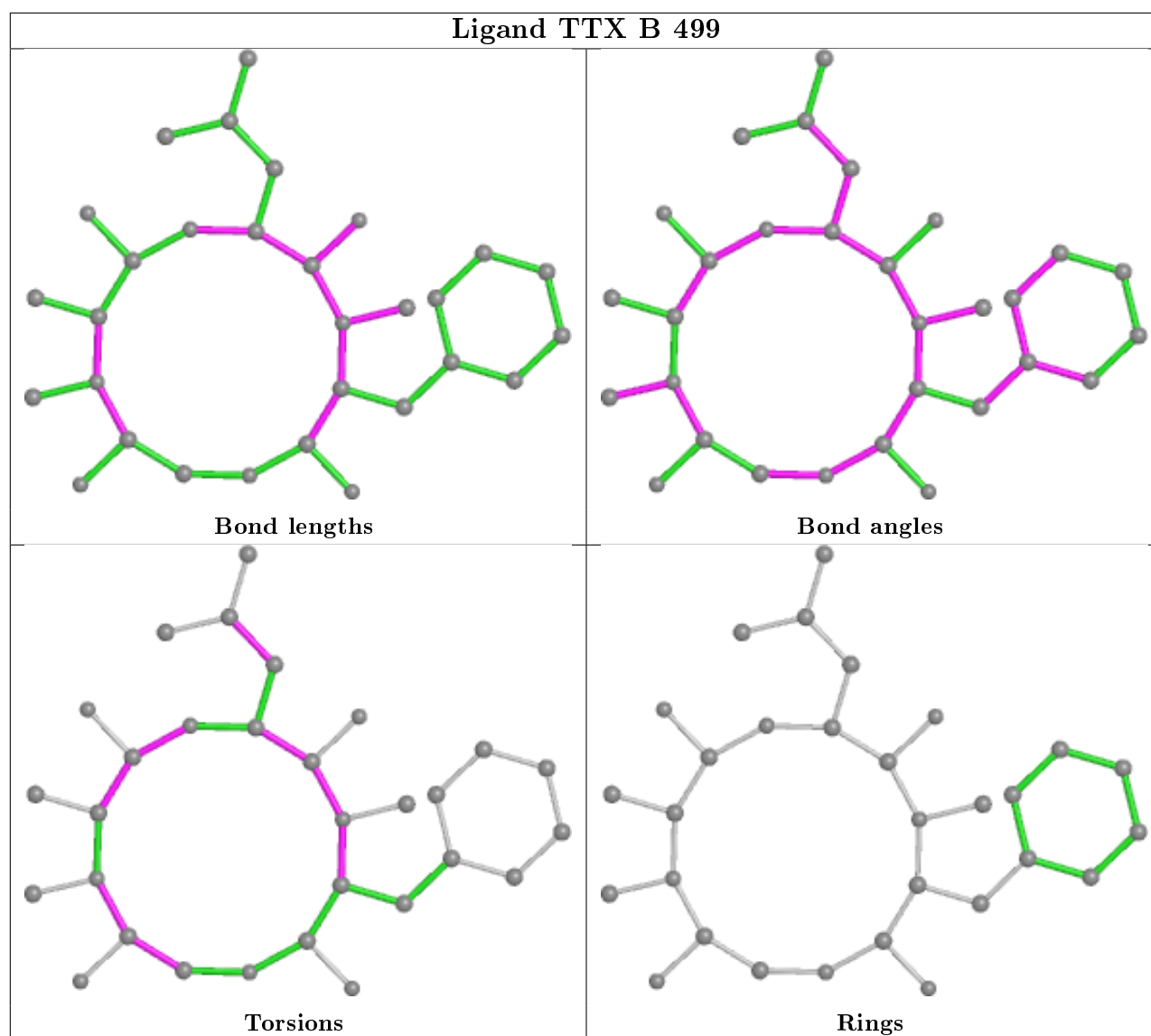
Mol	Chain	Res	Type	Atoms
3	B	499	TTX	C14-C15-N1-C6
3	B	499	TTX	O1-C6-N1-C7
3	B	499	TTX	C5-C6-N1-C7
3	B	499	TTX	C5-C6-N1-C15
3	B	499	TTX	O2-C8-N2-C5

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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.