

# wwPDB X-ray Structure Validation Summary Report (i)

Jan 27, 2024 – 11:59 AM EST

PDB ID : 1A79

Title : CRYSTAL STRUCTURE OF THE TRNA SPLICING ENDONUCLEASE

FROM METHANOCOCCUS JANNASCHII

Authors : Li, H.; Trotta, C.R.; Abelson, J.N.

Deposited on : 1998-03-23

Resolution : 2.28 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 (i) 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 (i)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : NOT EXECUTED EDS : NOT EXECUTED

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)

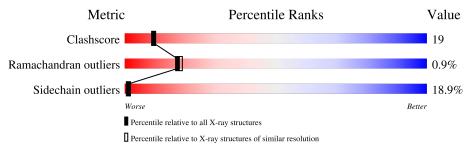
Validation Pipeline (wwPDB-VP) : 2.36

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality	Quality of chain					
1	A	171	53%	37%	10% •				
1	В	171	56%	35%	9%				
1	С	171	50%	40%	10%				
1	D	171	63%	27%	9% •				



## 2 Entry composition (i)

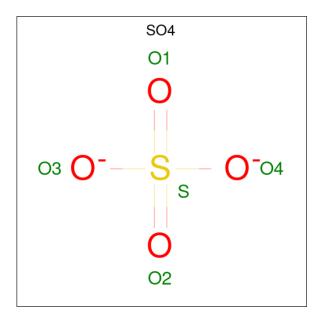
There are 4 unique types of molecules in this entry. The entry contains 5651 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TRNA ENDONUCLEASE.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	٨	171	Total	С	N	О	S	0	0	0
1	A	1/1	1396	908	231	255	2	0	U	U
1	В	171	Total	С	N	О	S	0	0	0
1	Б	111	1396	908	231	255	2	0	U	U
1	С	171	Total	С	N	О	S	0	0	0
1		111	1396	908	231	255	2	0	U	U
1	D	171	Total	С	N	О	S	0	0	0
1	.   D	D   171	1396	908	231	255	2		0	U

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mo	l	Chain	Residues	Atoms	ZeroOcc	AltConf
2		A	1	Total O S 5 4 1	0	0
2		С	1	Total O S 5 4 1	0	0



• Molecule 3 is GOLD ION (three-letter code: AU) (formula: Au).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Au 1 1	0	0
3	В	1	Total Au 1 1	0	0
3	С	1	Total Au 1 1	0	0
3	D	1	Total Au 1 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	12	Total O 12 12	0	0
4	В	14	Total O 14 14	0	0
4	С	14	Total O 14 14	0	0
4	D	13	Total O 13 13	0	0

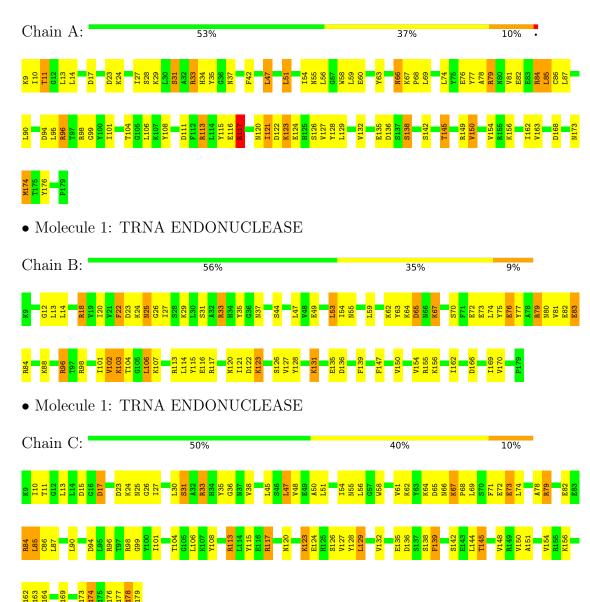


# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

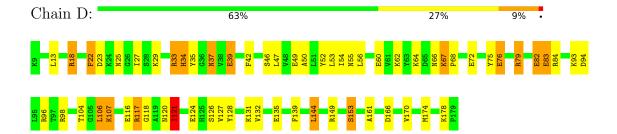
Note EDS was not executed.

• Molecule 1: TRNA ENDONUCLEASE



• Molecule 1: TRNA ENDONUCLEASE







# 4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	61.95Å 80.04Å 193.59Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	50.00 - 2.28	Depositor	
% Data completeness	77.2 (50.00-2.28)	Depositor	
(in resolution range)	11.2 (90.00 2.20)	Берозног	
$R_{merge}$	0.05	Depositor	
$R_{sym}$	0.05	Depositor	
Refinement program	X-PLOR 3.857	Depositor	
$R, R_{free}$	0.200 , $0.267$	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	5651	wwPDB-VP	
Average B, all atoms (Å <sup>2</sup> )	42.0	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: SO4, AU

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		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.37	0/1424	0.65	0/1920	
1	В	0.38	0/1424	0.62	0/1920	
1	С	0.37	0/1424	0.66	0/1920	
1	D	0.38	0/1424	0.63	1/1920 (0.1%)	
All	All	0.37	0/5696	0.64	1/7680 (0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	D	118	GLY	N-CA-C	5.02	125.65	113.10

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	1396	0	1419	71	0
1	В	1396	0	1419	55	0
1	С	1396	0	1419	74	0
1	D	1396	0	1419	42	0
2	A	5	0	0	0	0
2	С	5	0	0	0	0

Continued on next page...



Continued from previous page						
	$\mathcal{C}$	lontinued	l fr	rom	previous	page

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	В	1	0	0	0	0
3	С	1	0	0	0	0
3	D	1	0	0	0	0
4	A	12	0	0	0	0
4	В	14	0	0	1	0
4	С	14	0	0	0	0
4	D	13	0	0	0	0
All	All	5651	0	5676	217	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 19.

The worst 5 of 217 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:150:VAL:HG23	1:C:150:VAL:HG23	1.37	1.05	
1:A:120:ASN:ND2	1:A:123:LYS:H	1.57	1.02	
1:D:121:ILE:H	1:D:124:GLU:HG3	1.26	1.01	
1:A:120:ASN:HD21	1:A:123:LYS:H	1.17	0.87	
1:A:78:ALA:HB1	1:A:85:LEU:HD13	1.58	0.85	

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	Perce	entiles
1	A	169/171 (99%)	155 (92%)	12 (7%)	2 (1%)	13	12
1	В	$169/171 \ (99\%)$	158 (94%)	11 (6%)	0	100	100
1	С	169/171 (99%)	156 (92%)	13 (8%)	0	100	100

Continued on next page...



Continued from previous page...

Mol	Chain	Analysed Favoured		Allowed	Outliers	Percentiles
1	D	169/171 (99%)	155 (92%)	10 (6%)	4 (2%)	6 4
All	All	676/684 (99%)	624 (92%)	46 (7%)	6 (1%)	17 18

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	117	ARG
1	A	117	ARG
1	D	121	ILE
1	D	34	HIS
1	D	66	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	151/151 (100%)	121 (80%)	30 (20%)	1	1
1	В	151/151 (100%)	124 (82%)	27 (18%)	2	1
1	С	151/151 (100%)	121 (80%)	30 (20%)	1	1
1	D	151/151 (100%)	124 (82%)	27 (18%)	2	1
All	All	604/604 (100%)	490 (81%)	114 (19%)	1	1

5 of 114 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type	
1	С	11	THR	
1	D	135	GLU	
1	С	79	ARG	
1	D	131	LYS	
1	D	76	GLU	

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:



Mol	Chain	Res	Type
1	С	173	ASN
1	D	37	ASN
1	D	80	ASN
1	D	66	ASN
1	В	80	ASN

#### 5.3.3 RNA (i)

There are no RNA molecules 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 monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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		gles	
Moi   Type	Counts				RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
2	SO4	С	2	-	4,4,4	0.13	0	6,6,6	0.13	0
2	SO4	A	1	-	4,4,4	0.17	0	6,6,6	0.16	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.



No monomer is involved in short contacts.

## 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 (i)

#### 6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

#### 6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

