



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 6, 2016 – 11:10 AM EST

PDB ID : 5HC9  
Title : Thermotoga maritima CCA-adding enzyme complexed with tRNA\_CCA  
Authors : Yamashita, S.; Tomita, K.  
Deposited on : 2016-01-04  
Resolution : 2.90 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 : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028442

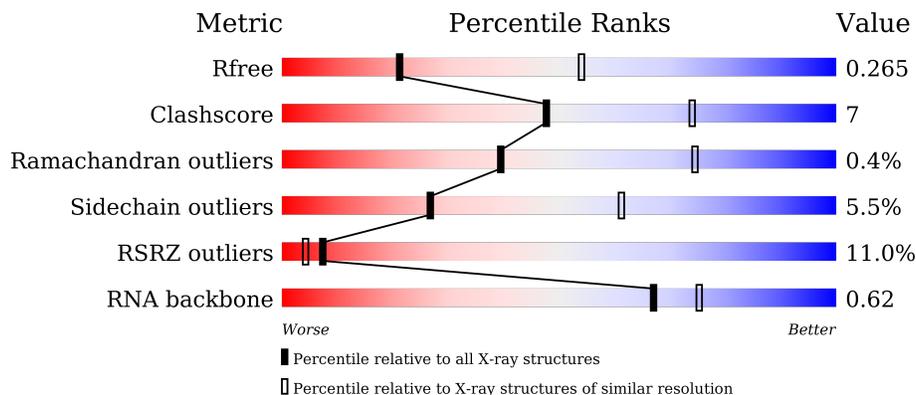
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)
RNA backbone	2183	1093 (3.30-2.50)

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.

Mol	Chain	Length	Quality of chain
1	A	441	 5% (poor fit), 73% (0-1 outliers), 20% (2-3 outliers), 2% (not modelled)
1	B	441	 5% (poor fit), 72% (0-1 outliers), 18% (2-3 outliers), 7% (not modelled)
2	C	76	 49% (poor fit), 57% (0-1 outliers), 37% (2-3 outliers), 7% (not modelled)
2	D	76	 32% (poor fit), 58% (0-1 outliers), 33% (2-3 outliers), 9% (not modelled)

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10128 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 nucleotidyl transferase-related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	425	3502	2264	591	636	11	0	0	0
1	B	410	3378	2183	575	610	10	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q9WZH4
A	429	LYS	-	expression tag	UNP Q9WZH4
A	430	LEU	-	expression tag	UNP Q9WZH4
A	431	ALA	-	expression tag	UNP Q9WZH4
A	432	ALA	-	expression tag	UNP Q9WZH4
A	433	ALA	-	expression tag	UNP Q9WZH4
A	434	LEU	-	expression tag	UNP Q9WZH4
A	435	GLU	-	expression tag	UNP Q9WZH4
A	436	HIS	-	expression tag	UNP Q9WZH4
A	437	HIS	-	expression tag	UNP Q9WZH4
A	438	HIS	-	expression tag	UNP Q9WZH4
A	439	HIS	-	expression tag	UNP Q9WZH4
A	440	HIS	-	expression tag	UNP Q9WZH4
A	441	HIS	-	expression tag	UNP Q9WZH4
B	1	MET	-	initiating methionine	UNP Q9WZH4
B	429	LYS	-	expression tag	UNP Q9WZH4
B	430	LEU	-	expression tag	UNP Q9WZH4
B	431	ALA	-	expression tag	UNP Q9WZH4
B	432	ALA	-	expression tag	UNP Q9WZH4
B	433	ALA	-	expression tag	UNP Q9WZH4
B	434	LEU	-	expression tag	UNP Q9WZH4
B	435	GLU	-	expression tag	UNP Q9WZH4
B	436	HIS	-	expression tag	UNP Q9WZH4
B	437	HIS	-	expression tag	UNP Q9WZH4
B	438	HIS	-	expression tag	UNP Q9WZH4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	439	HIS	-	expression tag	UNP Q9WZH4
B	440	HIS	-	expression tag	UNP Q9WZH4
B	441	HIS	-	expression tag	UNP Q9WZH4

- Molecule 2 is a RNA chain called tRNAphe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	76	1623	723	291	533	76	0	0	0
2	D	76	1623	723	291	533	76	0	0	0

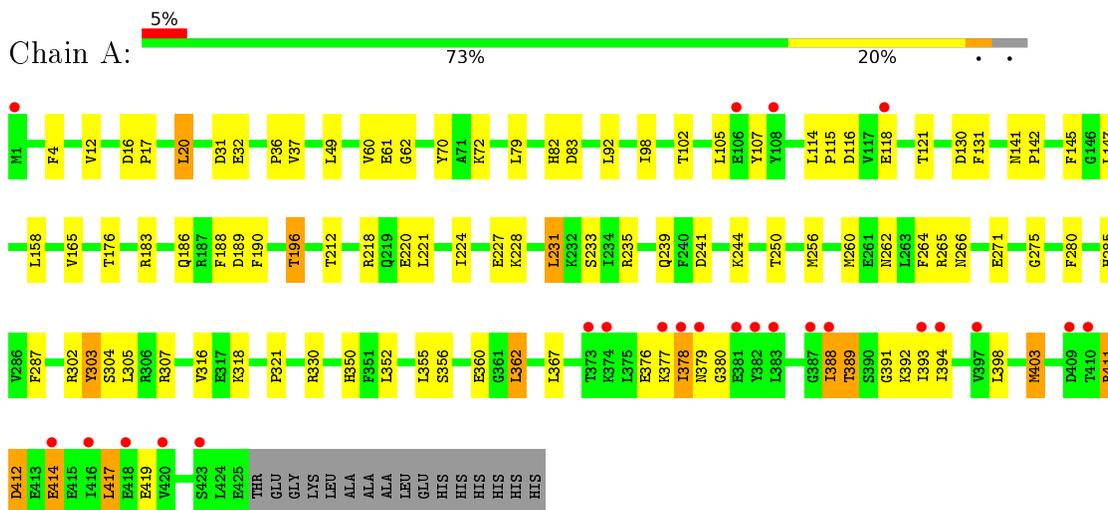
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

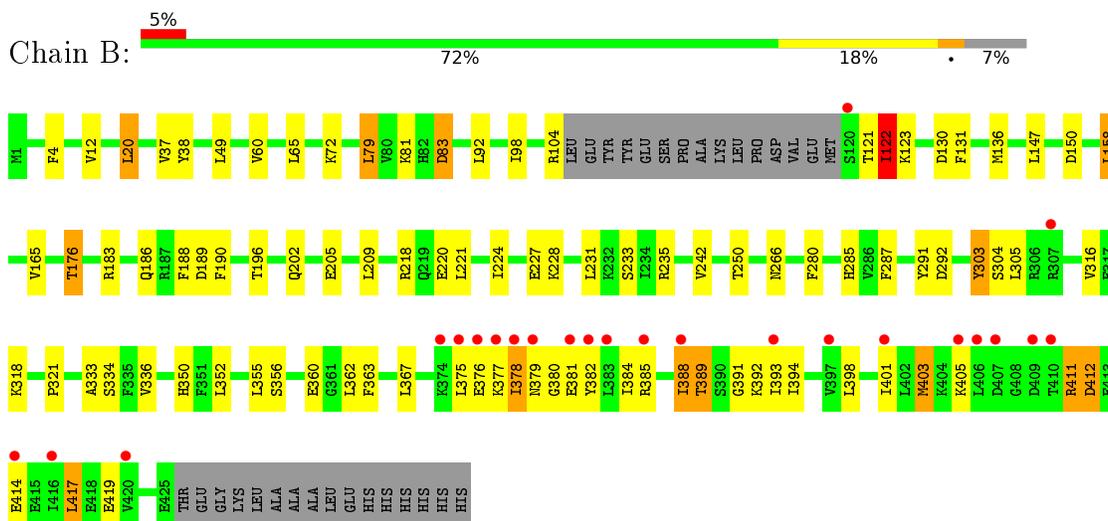
### 3 Residue-property plots

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.

- Molecule 1: tRNA nucleotidyl transferase-related protein

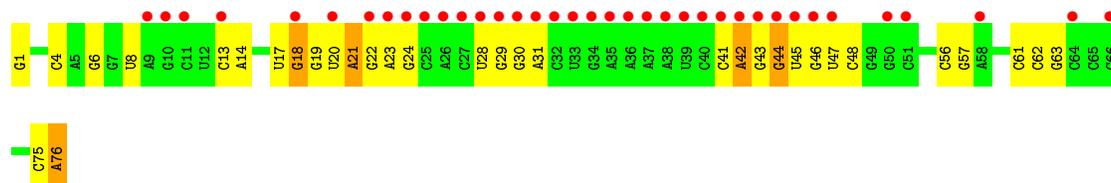


- Molecule 1: tRNA nucleotidyl transferase-related protein

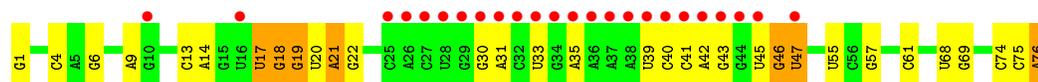


- Molecule 2: tRNA<sup>phe</sup>





- Molecule 2: tRNAphe



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.18Å 96.19Å 108.58Å 90.00° 110.30° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 48.78 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.90) 99.7 (48.78-2.90)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 2.91Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.215 , 0.264 0.220 , 0.265	Depositor DCC
$R_{free}$ test set	2103 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	69.4	Xtrriage
Anisotropy	0.396	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 74.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10128	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	132.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: MG

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	0.23	0/3568	0.42	0/4798
1	B	0.23	0/3439	0.42	0/4620
2	C	0.28	1/1813 (0.1%)	0.67	0/2823
2	D	0.28	1/1813 (0.1%)	0.67	0/2823
All	All	0.25	2/10633 (0.0%)	0.53	0/15064

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	G	OP3-P	-10.57	1.48	1.61
2	D	1	G	OP3-P	-10.43	1.48	1.61

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	412	ASP	Peptide
1	B	412	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	B	83	ASP	Peptide

## 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	3502	0	3596	58	0
1	B	3378	0	3478	53	0
2	C	1623	0	822	18	0
2	D	1623	0	822	19	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	10128	0	8718	140	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 7.

The worst 5 of 140 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:218:ARG:NH2	1:A:304:SER:O	2.24	0.71
1:A:411:ARG:NH2	1:A:419:GLU:OE2	2.26	0.69
1:B:12:VAL:HA	1:B:20:LEU:HD11	1.74	0.68
1:A:379:ASN:ND2	2:C:56:C:OP1	2.27	0.67
1:A:32:GLU:OE2	1:A:70:TYR:OH	2.10	0.66

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	423/441 (96%)	398 (94%)	24 (6%)	1 (0%)	52	84
1	B	406/441 (92%)	382 (94%)	22 (5%)	2 (0%)	34	71
All	All	829/882 (94%)	780 (94%)	46 (6%)	3 (0%)	39	74

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	122	ILE
1	A	378	ILE
1	B	378	ILE

### 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	383/395 (97%)	361 (94%)	22 (6%)	25	59
1	B	369/395 (93%)	350 (95%)	19 (5%)	29	65
All	All	752/790 (95%)	711 (94%)	41 (6%)	27	61

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	411	ARG
1	B	20	LEU
1	B	403	MET
1	A	412	ASP
1	A	414	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	75/76 (98%)	15 (20%)	3 (4%)
2	D	75/76 (98%)	14 (18%)	4 (5%)
All	All	150/152 (98%)	29 (19%)	7 (4%)

5 of 29 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	6	G
2	C	13	C
2	C	17	U
2	C	18	G
2	C	19	G

5 of 7 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	D	19	G
2	D	46	G
2	D	21	A
2	C	21	A
2	D	45	U

## 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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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

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 [i](#)

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

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	425/441 (96%)	0.56	24 (5%) 28 21	48, 82, 210, 261	0
1	B	410/441 (92%)	0.52	24 (5%) 26 19	48, 79, 188, 278	0
2	C	76/76 (100%)	2.51	37 (48%) 0 0	99, 221, 341, 369	0
2	D	76/76 (100%)	1.53	24 (31%) 1 0	61, 185, 327, 342	0
All	All	987/1034 (95%)	0.77	109 (11%) 7 4	48, 88, 248, 369	0

The worst 5 of 109 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	34	G	11.0
1	B	388	ILE	9.3
2	C	35	A	9.0
2	C	37	A	8.0
2	C	40	C	7.7

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	B	1001	1/1	0.95	0.42	-	71,71,71,71	0
3	MG	A	1001	1/1	0.86	0.36	-	62,62,62,62	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.