



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 03:50 am BST

PDB ID : 3UGT  
Title : Crystal structure of the yeast mitochondrial threonyl-tRNA synthetase - orthorhombic crystal form  
Authors : Peterson, K.M.; Ling, J.; Simonovic, I.; Cho, C.; Soll, D.; Simonovic, M.  
Deposited on : 2011-11-02  
Resolution : 3.60 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  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

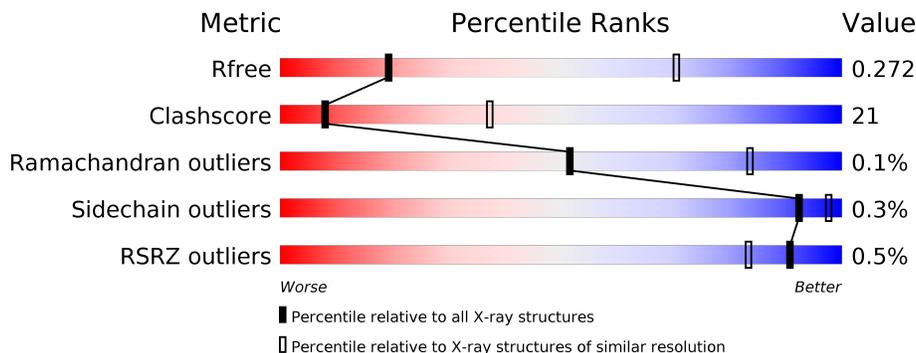
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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))
$R_{free}$	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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 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  $\leq 5\%$ . 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	460	
1	B	460	
1	C	460	
1	D	460	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13459 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 Threonyl-tRNA synthetase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	419	Total 3397	C 2195	N 571	O 613	S 18	0	3	0
1	B	419	Total 3285	C 2115	N 553	O 601	S 16	3	4	0
1	C	427	Total 3432	C 2206	N 574	O 634	S 18	1	2	0
1	D	418	Total 3295	C 2121	N 552	O 605	S 17	0	1	0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	MET	-	EXPRESSION TAG	UNP P07236
A	4	GLY	-	EXPRESSION TAG	UNP P07236
A	5	SER	-	EXPRESSION TAG	UNP P07236
A	6	SER	-	EXPRESSION TAG	UNP P07236
A	7	HIS	-	EXPRESSION TAG	UNP P07236
A	8	HIS	-	EXPRESSION TAG	UNP P07236
A	9	HIS	-	EXPRESSION TAG	UNP P07236
A	10	HIS	-	EXPRESSION TAG	UNP P07236
A	11	HIS	-	EXPRESSION TAG	UNP P07236
A	12	HIS	-	EXPRESSION TAG	UNP P07236
A	13	SER	-	EXPRESSION TAG	UNP P07236
A	14	SER	-	EXPRESSION TAG	UNP P07236
A	15	GLY	-	EXPRESSION TAG	UNP P07236
A	16	LEU	-	EXPRESSION TAG	UNP P07236
A	17	VAL	-	EXPRESSION TAG	UNP P07236
A	18	PRO	-	EXPRESSION TAG	UNP P07236
A	19	ARG	-	EXPRESSION TAG	UNP P07236
A	20	GLY	-	EXPRESSION TAG	UNP P07236
A	21	SER	-	EXPRESSION TAG	UNP P07236
A	22	HIS	-	EXPRESSION TAG	UNP P07236
A	23	MET	-	EXPRESSION TAG	UNP P07236

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Chain	Residue	Modelled	Actual	Comment	Reference
A	24	ALA	-	EXPRESSION TAG	UNP P07236
A	25	SER	-	EXPRESSION TAG	UNP P07236
B	3	MET	-	EXPRESSION TAG	UNP P07236
B	4	GLY	-	EXPRESSION TAG	UNP P07236
B	5	SER	-	EXPRESSION TAG	UNP P07236
B	6	SER	-	EXPRESSION TAG	UNP P07236
B	7	HIS	-	EXPRESSION TAG	UNP P07236
B	8	HIS	-	EXPRESSION TAG	UNP P07236
B	9	HIS	-	EXPRESSION TAG	UNP P07236
B	10	HIS	-	EXPRESSION TAG	UNP P07236
B	11	HIS	-	EXPRESSION TAG	UNP P07236
B	12	HIS	-	EXPRESSION TAG	UNP P07236
B	13	SER	-	EXPRESSION TAG	UNP P07236
B	14	SER	-	EXPRESSION TAG	UNP P07236
B	15	GLY	-	EXPRESSION TAG	UNP P07236
B	16	LEU	-	EXPRESSION TAG	UNP P07236
B	17	VAL	-	EXPRESSION TAG	UNP P07236
B	18	PRO	-	EXPRESSION TAG	UNP P07236
B	19	ARG	-	EXPRESSION TAG	UNP P07236
B	20	GLY	-	EXPRESSION TAG	UNP P07236
B	21	SER	-	EXPRESSION TAG	UNP P07236
B	22	HIS	-	EXPRESSION TAG	UNP P07236
B	23	MET	-	EXPRESSION TAG	UNP P07236
B	24	ALA	-	EXPRESSION TAG	UNP P07236
B	25	SER	-	EXPRESSION TAG	UNP P07236
C	3	MET	-	EXPRESSION TAG	UNP P07236
C	4	GLY	-	EXPRESSION TAG	UNP P07236
C	5	SER	-	EXPRESSION TAG	UNP P07236
C	6	SER	-	EXPRESSION TAG	UNP P07236
C	7	HIS	-	EXPRESSION TAG	UNP P07236
C	8	HIS	-	EXPRESSION TAG	UNP P07236
C	9	HIS	-	EXPRESSION TAG	UNP P07236
C	10	HIS	-	EXPRESSION TAG	UNP P07236
C	11	HIS	-	EXPRESSION TAG	UNP P07236
C	12	HIS	-	EXPRESSION TAG	UNP P07236
C	13	SER	-	EXPRESSION TAG	UNP P07236
C	14	SER	-	EXPRESSION TAG	UNP P07236
C	15	GLY	-	EXPRESSION TAG	UNP P07236
C	16	LEU	-	EXPRESSION TAG	UNP P07236
C	17	VAL	-	EXPRESSION TAG	UNP P07236
C	18	PRO	-	EXPRESSION TAG	UNP P07236
C	19	ARG	-	EXPRESSION TAG	UNP P07236

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Chain	Residue	Modelled	Actual	Comment	Reference
C	20	GLY	-	EXPRESSION TAG	UNP P07236
C	21	SER	-	EXPRESSION TAG	UNP P07236
C	22	HIS	-	EXPRESSION TAG	UNP P07236
C	23	MET	-	EXPRESSION TAG	UNP P07236
C	24	ALA	-	EXPRESSION TAG	UNP P07236
C	25	SER	-	EXPRESSION TAG	UNP P07236
D	3	MET	-	EXPRESSION TAG	UNP P07236
D	4	GLY	-	EXPRESSION TAG	UNP P07236
D	5	SER	-	EXPRESSION TAG	UNP P07236
D	6	SER	-	EXPRESSION TAG	UNP P07236
D	7	HIS	-	EXPRESSION TAG	UNP P07236
D	8	HIS	-	EXPRESSION TAG	UNP P07236
D	9	HIS	-	EXPRESSION TAG	UNP P07236
D	10	HIS	-	EXPRESSION TAG	UNP P07236
D	11	HIS	-	EXPRESSION TAG	UNP P07236
D	12	HIS	-	EXPRESSION TAG	UNP P07236
D	13	SER	-	EXPRESSION TAG	UNP P07236
D	14	SER	-	EXPRESSION TAG	UNP P07236
D	15	GLY	-	EXPRESSION TAG	UNP P07236
D	16	LEU	-	EXPRESSION TAG	UNP P07236
D	17	VAL	-	EXPRESSION TAG	UNP P07236
D	18	PRO	-	EXPRESSION TAG	UNP P07236
D	19	ARG	-	EXPRESSION TAG	UNP P07236
D	20	GLY	-	EXPRESSION TAG	UNP P07236
D	21	SER	-	EXPRESSION TAG	UNP P07236
D	22	HIS	-	EXPRESSION TAG	UNP P07236
D	23	MET	-	EXPRESSION TAG	UNP P07236
D	24	ALA	-	EXPRESSION TAG	UNP P07236
D	25	SER	-	EXPRESSION TAG	UNP P07236

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	A	18	Total 18	O 18	0	0
3	B	7	Total 7	O 7	0	0
3	C	15	Total 15	O 15	0	0
3	D	6	Total 6	O 6	0	0





P454  
I485  
E486  
I487  
K462

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.08Å 157.94Å 237.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.11 – 3.60 35.11 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.5 (35.11-3.60) 95.3 (35.11-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 3.48Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.237 , 0.275 0.231 , 0.272	Depositor DCC
$R_{free}$ test set	1750 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	89.8	Xtrriage
Anisotropy	0.400	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 37.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.016 for -k,-h,-l	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	13459	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% 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

### 5.1 Standard geometry

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

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	0.22	0/3494	0.40	0/4729
1	B	0.22	0/3372	0.41	0/4574
1	C	0.23	0/3529	0.41	0/4786
1	D	0.22	0/3380	0.41	0/4590
All	All	0.22	0/13775	0.41	0/18679

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	1
1	C	0	3
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	439	ARG	Peptide
1	B	62	LEU	Peptide
1	C	132	ASN	Peptide
1	C	296	GLN	Peptide
1	C	297	LEU	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	3397	0	3262	130	0
1	B	3285	0	3069	156	0
1	C	3432	0	3241	136	0
1	D	3295	0	3062	167	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	18	0	0	0	0
3	B	7	0	0	0	0
3	C	15	0	0	0	0
3	D	6	0	0	0	0
All	All	13459	0	12634	556	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 21.

The worst 5 of 556 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:C:119:THR:H	1:C:120:ASP:HA	1.28	0.98
1:C:296:GLN:HA	1:C:298:PRO:HD2	1.46	0.97
1:B:269:PHE:HB2	1:B:270:TYR:HA	1.50	0.92
1:C:92:PRO:HB3	1:D:58:SER:HB3	1.53	0.90
1:D:40:SER:O	1:D:44:GLN:HB2	1.73	0.87

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	415/460 (90%)	377 (91%)	37 (9%)	1 (0%)	47	79
1	B	415/460 (90%)	368 (89%)	46 (11%)	1 (0%)	47	79
1	C	426/460 (93%)	390 (92%)	36 (8%)	0	100	100
1	D	412/460 (90%)	370 (90%)	42 (10%)	0	100	100
All	All	1668/1840 (91%)	1505 (90%)	161 (10%)	2 (0%)	51	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	394	VAL
1	A	394	VAL

### 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	362/416 (87%)	361 (100%)	1 (0%)	92	97
1	B	335/416 (80%)	333 (99%)	2 (1%)	86	94
1	C	364/416 (88%)	363 (100%)	1 (0%)	92	97
1	D	338/416 (81%)	338 (100%)	0	100	100
All	All	1399/1664 (84%)	1395 (100%)	4 (0%)	92	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	LEU
1	B	62	LEU
1	B	341	TRP
1	C	320	ARG

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

sidechains are listed below:

Mol	Chain	Res	Type
1	B	393	ASN
1	C	132	ASN
1	D	308	GLN
1	B	414	ASN
1	B	429[A]	GLN

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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 [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](#)

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	419/460 (91%)	-0.50	0 <b>100</b> <b>100</b>	64, 83, 110, 132	0
1	B	419/460 (91%)	-0.31	6 (1%) 75 61	64, 98, 138, 149	1 (0%)
1	C	427/460 (92%)	-0.43	0 <b>100</b> <b>100</b>	57, 79, 105, 115	3 (0%)
1	D	418/460 (90%)	-0.35	2 (0%) 91 83	64, 93, 126, 137	1 (0%)
All	All	1683/1840 (91%)	-0.40	8 (0%) 91 83	57, 88, 125, 149	5 (0%)

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	238	ASP	2.8
1	B	237	GLY	2.7
1	B	243	ASN	2.5
1	B	239	LEU	2.5
1	B	36	ALA	2.3

### 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	B	2	1/1	0.91	0.27	92,92,92,92	0
2	ZN	D	463	1/1	0.93	0.21	103,103,103,103	0
2	ZN	C	463	1/1	0.97	0.23	59,59,59,59	0
2	ZN	A	1	1/1	0.98	0.23	70,70,70,70	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.