



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:24 PM GMT

PDB ID : 3TUP  
Title : Crystal structure of human mitochondrial PheRS complexed with tRNAPhe  
in the active open state  
Authors : Safro, M.; Klipcan, L.; Moor, N.; Finarov, I.; Kessler, N.; Sukhanova, M.  
Deposited on : 2011-09-17  
Resolution : 3.05 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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

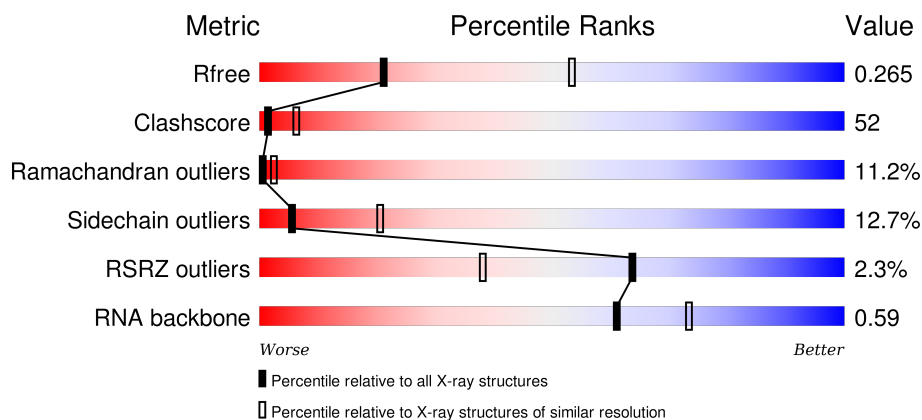
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

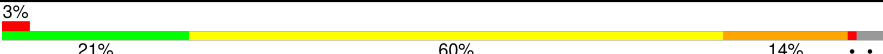

The reported resolution of this entry is 3.05 Å.

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	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (3.10-3.02)
RNA backbone	2183	1035 (3.50-2.62)

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	415	
2	T	76	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4928 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 Phenylalanyl-tRNA synthetase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	0	0
			3347	2143	592	600	12			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP O95363

- Molecule 2 is a RNA chain called Thermus thermophilus tRNAPhe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	74	Total	C	N	O	P	0	0	0
			1581	704	281	522	74			



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.04Å 116.04Å 123.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.94 – 3.05 46.53 – 3.05	Depositor EDS
% Data completeness (in resolution range)	(Not available) (38.94-3.05) 99.5 (46.53-3.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.51 (at 3.06Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.245 , 0.295 0.257 , 0.265	Depositor DCC
$R_{free}$ test set	923 reflections (4.96%)	DCC
Wilson B-factor (Å <sup>2</sup> )	93.0	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 62.9	EDS
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 18651 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4928	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.50	1/3439 (0.0%)	0.75	1/4655 (0.0%)
2	T	0.55	1/1766 (0.1%)	0.82	4/2750 (0.1%)
All	All	0.52	2/5205 (0.0%)	0.78	5/7405 (0.1%)

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
2	T	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	1	G	OP3-P	-6.29	1.53	1.61
1	A	365	LYS	CD-CE	5.02	1.63	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	18	G	N9-C1'-C2'	6.58	122.55	114.00
2	T	19	G	N9-C1'-C2'	6.40	122.31	114.00
2	T	46	G	N9-C1'-C2'	6.28	122.17	114.00
1	A	365	LYS	CD-CE-NZ	5.88	125.21	111.70
2	T	58	A	N9-C1'-C2'	5.43	121.06	114.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	T	18	G	Sidechain

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Mol	Chain	Res	Type	Group
2	T	46	G	Sidechain

## 5.2 Too-close contacts ⓘ

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	3347	0	3254	427	0
2	T	1581	0	798	45	0
All	All	4928	0	4052	468	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 52.

The worst 5 of 468 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:68:ARG:HG3	1:A:69:PHE:H	1.29	0.98
1:A:236:HIS:HB3	1:A:237:PRO:HD3	1.44	0.98
1:A:405:ALA:HA	1:A:409:LEU:HD12	1.44	0.97
1:A:389:LEU:H	1:A:389:LEU:HD23	1.30	0.96
1:A:182:PHE:HA	1:A:196:THR:HG23	1.47	0.94

There are no symmetry-related clashes.

## 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	402/415 (97%)	279 (69%)	78 (19%)	45 (11%)	0 2

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	PRO
1	A	25	ASP
1	A	46	GLN
1	A	69	PHE
1	A	101	SER

### 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	363/370 (98%)	317 (87%)	46 (13%)	5 20

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	HIS
1	A	240	GLU
1	A	381	THR
1	A	203	VAL
1	A	223	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	GLN
1	A	151	HIS
1	A	329	ASN
1	A	146	GLN
1	A	339	ASN



### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	T	73/76 (96%)	17 (23%)	8 (10%)

5 of 17 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	T	7	G
2	T	8	U
2	T	9	A
2	T	10	G
2	T	13	C

5 of 8 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	T	22	G
2	T	60	U
2	T	47	U
2	T	19	G
2	T	46	G

## 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](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

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	404/415 (97%)	0.04	11 (2%) 58 32	50, 87, 118, 120	0
2	T	74/76 (97%)	0.21	0 100 100	79, 105, 120, 120	0
All	All	478/491 (97%)	0.06	11 (2%) 64 38	50, 90, 119, 120	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	247	GLY	4.1
1	A	248	GLU	4.0
1	A	222	GLU	3.1
1	A	223	LEU	2.8
1	A	245	PHE	2.6

### 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](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.