



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 2, 2023 – 04:28 PM EDT

PDB ID : 6NLY
Title : Fragment of human mitochondrial Alanyl-tRNA Synthetase C-Ala domain
Authors : Kuhle, B.; Schimmel, P.
Deposited on : 2019-01-09
Resolution : 2.31 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : **FAILED**
Xtrriage (Phenix) : 1.13
EDS : **FAILED**
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) : 2.35.1

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 2.31 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 5425 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 Alanine-tRNA ligase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	178	1339	836	244	249	10	0	0	0
1	A	181	1357	847	247	253	10	0	0	0
1	C	176	1324	827	240	247	10	0	0	0
1	D	182	1384	863	258	253	10	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	986	LEU	-	expression tag	UNP Q5J TZ9
B	987	GLU	-	expression tag	UNP Q5J TZ9
B	988	HIS	-	expression tag	UNP Q5J TZ9
B	989	HIS	-	expression tag	UNP Q5J TZ9
B	990	HIS	-	expression tag	UNP Q5J TZ9
B	991	HIS	-	expression tag	UNP Q5J TZ9
B	992	HIS	-	expression tag	UNP Q5J TZ9
B	993	HIS	-	expression tag	UNP Q5J TZ9
A	986	LEU	-	expression tag	UNP Q5J TZ9
A	987	GLU	-	expression tag	UNP Q5J TZ9
A	988	HIS	-	expression tag	UNP Q5J TZ9
A	989	HIS	-	expression tag	UNP Q5J TZ9
A	990	HIS	-	expression tag	UNP Q5J TZ9
A	991	HIS	-	expression tag	UNP Q5J TZ9
A	992	HIS	-	expression tag	UNP Q5J TZ9
A	993	HIS	-	expression tag	UNP Q5J TZ9
C	986	LEU	-	expression tag	UNP Q5J TZ9
C	987	GLU	-	expression tag	UNP Q5J TZ9
C	988	HIS	-	expression tag	UNP Q5J TZ9
C	989	HIS	-	expression tag	UNP Q5J TZ9
C	990	HIS	-	expression tag	UNP Q5J TZ9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	991	HIS	-	expression tag	UNP Q5JTZ9
C	992	HIS	-	expression tag	UNP Q5JTZ9
C	993	HIS	-	expression tag	UNP Q5JTZ9
D	986	LEU	-	expression tag	UNP Q5JTZ9
D	987	GLU	-	expression tag	UNP Q5JTZ9
D	988	HIS	-	expression tag	UNP Q5JTZ9
D	989	HIS	-	expression tag	UNP Q5JTZ9
D	990	HIS	-	expression tag	UNP Q5JTZ9
D	991	HIS	-	expression tag	UNP Q5JTZ9
D	992	HIS	-	expression tag	UNP Q5JTZ9
D	993	HIS	-	expression tag	UNP Q5JTZ9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	5	Total O 5 5	0	0
2	A	6	Total O 6 6	0	0
2	C	4	Total O 4 4	0	0
2	D	6	Total O 6 6	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	103.22Å 317.23Å 54.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.02 – 2.31	Depositor
% Data completeness (in resolution range)	99.1 (38.02-2.31)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.27 (at 2.31Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.209 , 0.257	Depositor
Wilson B-factor (Å ²)	50.2	Xtrriage
Anisotropy	0.848	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	5425	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.11 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.5256e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.